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L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:115107 HCAPLUS
 DOCUMENT NUMBER: 134:178271
 TITLE: Process for preparing substituted cyclohexanoic acids
 via α -chloroepoxy esters
 INVENTOR(S): Diederich, Ann M.; Novak, Vance J.
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
 SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010822	A1	20010215	WO 2000-US21394	20000804
W:			AE, AL, AU, BA, BB, BG, BR, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	
BR 2000013025	A	20020416	BR 2000-13025	20000804
EP 1200394	A1	20020502	EP 2000-953844	20000804
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL	
JP 2003506431	T2	20030218	JP 2001-515289	20000804
ZA 2002000965	A	20030204	ZA 2002-965	20020204
NO 2002000561	A	20020205	NO 2002-561	20020205
PRIORITY APPLN. INFO.:			US 1999-147576P P 19990806	
			WO 2000-US21394 W 20000804	
OTHER SOURCE(S):		CASREACT 134:178271; MARPAT 134:178271		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

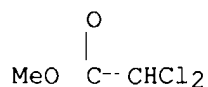
AB A process for preparing substituted cyclohexanoic acids I is proposed, where Ra is a carbon-containing group optionally linked by oxygen, sulfur or nitrogen to the cyclohexyl ring and n is 1-10; and R and R* are independently but not simultaneously hydrogen or C(O)E where E is OR14 or SR14, where R14 is hydrogen or alkyl of 1-6 carbon atoms; which process comprises treating an epoxide II with DMSO and an alkali metal salt, wherein E is OR14 or SR14, where R14 is hydrogen or alkyl of 1-6 carbon atoms; Ra is the same as defined for I; and Y is Br, Cl, F or I. Thus, α -chloroepoxy ester III was prepared via reaction of 4-cyano-4-(3-cyclopentyloxy-4-methoxyphenyl)cyclohexan-1-one with Me dichloroacetate and tert-butoxide in THF, subsequently saponified and the corresponding chloroepoxy acid treated with DMSO, NaCl and water, and heated to 150 °C for 3.5 h to yield IV (59%).

IT **116-54-1**, Methyl dichloroacetate **152630-47-2**, 4-Cyano-4-(3-cyclopentyloxy-4-methoxyphenyl)cyclohexan-1-one
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (epoxide formation and subsequent esterification; process for preparing

substituted cyclohexanoic acids via α - **chloroepoxy**
esters)

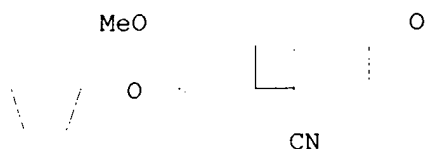
RN 116-54-1 HCAPLUS

CN Acetic acid, dichloro-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 152630-47-2 HCAPLUS

CN Cyclohexanecarbonitrile, 1-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-oxo-
(9CI) (CA INDEX NAME)



IT 153259-65-5P

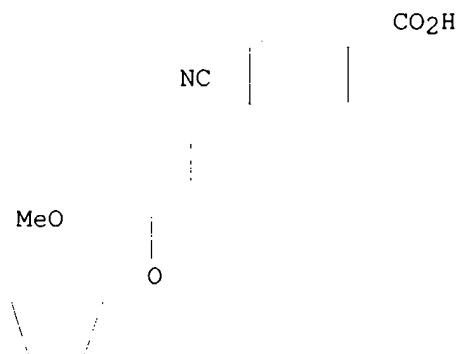
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP
(Preparation)

(process for preparing substituted cyclohexanoic acids via α -
chloroepoxy esters)

RN 153259-65-5 HCAPLUS

CN Cyclohexanecarboxylic acid, 4-cyano-4-[3-(cyclopentyloxy)-4-methoxyphenyl]-
, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 67-68-5, DMSO, reactions 535-15-9, Ethyl dichloroacetate

865-47-4 7447-40-7, Potassium chloride, reactions

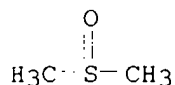
7447-41-8, Lithium chloride, reactions 7647-14-5, Sodium
chloride, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

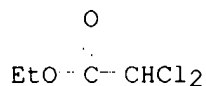
(process for preparing substituted cyclohexanoic acids via α -
chloroepoxy esters)

RN 67-68-5 HCAPLUS

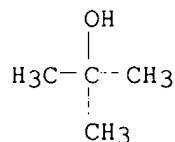
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)



RN 535-15-9 HCAPLUS
 CN Acetic acid, dichloro-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 865-47-4 HCAPLUS
 CN 2-Propanol, 2-methyl-, potassium salt (9CI) (CA INDEX NAME)



● K

RN 7447-40-7 HCAPLUS
 CN Potassium chloride (KCl) (9CI) (CA INDEX NAME)

Cl K

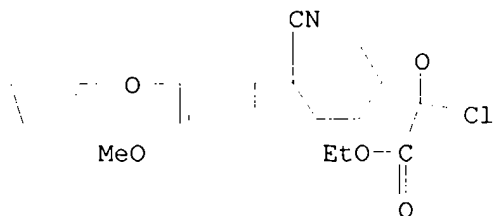
RN 7447-41-8 HCAPLUS
 CN Lithium chloride (LiCl) (9CI) (CA INDEX NAME)

Cl⁻ Li

RN 7647-14-5 HCAPLUS
 CN Sodium chloride (NaCl) (9CI) (CA INDEX NAME)

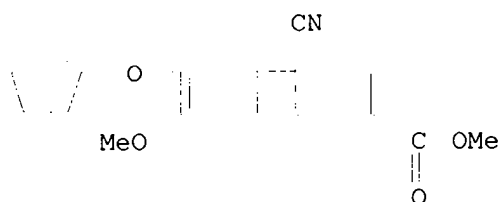
Cl⁻ Na

IT **326009-01-2P 326009-02-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (process for preparing substituted cyclohexanoic acids via α-
chloroepoxy esters)
 RN 326009-01-2 HCAPLUS
 CN 1-Oxaspiro[2.5]octane-2-carboxylic acid, 2-chloro-6-cyano-6-[3-
 (cyclopentyloxy)-4-methoxyphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 326009-02-3 HCAPLUS

CN Cyclohexanecarboxylic acid, 4-cyano-4-[3-(cyclopentyloxy)-4-methoxyphenyl]-, methyl ester (9CI) (CA INDEX NAME)



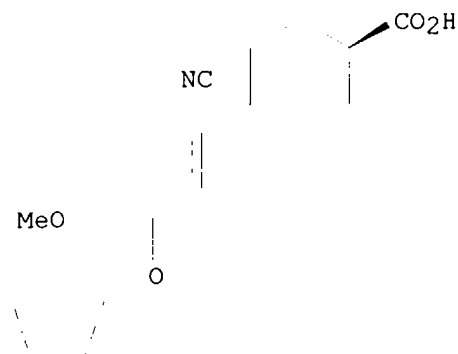
IT 153259-69-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparing substituted cyclohexanoic acids via α -chloroepoxy esters)

RN 153259-69-9 HCAPLUS

CN Cyclohexanecarboxylic acid, 4-cyano-4-[3-(cyclopentyloxy)-4-methoxyphenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

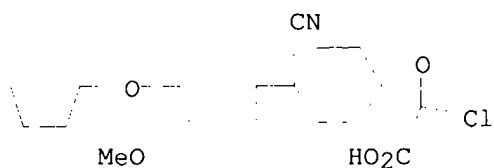


IT 326009-00-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparing substituted cyclohexanoic via α -chloroepoxy esters)

RN 326009-00-1 HCAPLUS

CN 1-Oxaspiro[2.5]octane-2-carboxylic acid, 2-chloro-6-cyano-6-[3-(cyclopentyloxy)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)



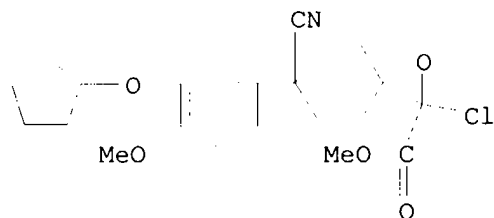
IT 326008-99-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(saponification; process for preparing substituted cyclohexanoic acids via α -chloroepoxy esters)

RN 326008-99-5 HCAPLUS

CN 1-Oxaspiro[2.5]octane-2-carboxylic acid, 2-chloro-6-cyano-6-[3-(cyclopentyloxy)-4-methoxyphenyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT